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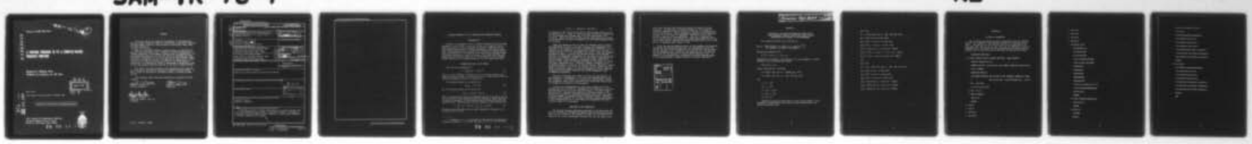

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A FORTRAN PROGRAM TO FIT A COMPLEX-VALUED TRANSFER FUNCTION

Richard C. McNee, M.S.
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This report has been reviewed by the Information Office (OI) and is releasable to the National Technical Information Service (NTIS). At NTIS, it will be available to the general public, including foreign nations.

This technical report has been reviewed and is approved for publication.

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20. ABSTRACT (Continue on reverse side if necessary and identify by block number)

A procedure is given to obtain the estimate of a transfer function with up to eight parameters (gain, delay, 3 zeros, and 3 poles). An example of a subroutine used in conjunction with a program for least-squares estimation of nonlinear parameters is included.

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A FORTRAN PROGRAM TO FIT A COMPLEX-VALUED TRANSFER FUNCTION

INTRODUCTION

A method is programmed to fit a transfer function with up to eight parameters: gain, delay, 3 leads (or zeros), and 3 lags (or poles). A modified version of a Fortran program by Donald W. Marquardt (1) for least-squares estimation of nonlinear parameters is the basic program used. The program requires a subroutine to define the residual and the partial derivatives of the function to be fitted and to evaluate these real-valued quantities at each of N points. This paper discusses the assumptions used and the structure of the subroutine to fit a complex valued function with a program written to fit real valued functions.

ASSUMPTIONS MADE IN THE METHOD

The norm to be minimized is:

$$\phi = \sum_{i=1}^{n} |H(j\omega_i) - \hat{H}(j\omega_i)|^2 \quad (1)$$

where ω is the frequency in radians, H is the observed value of the transfer function, and $\hat{H}$ is the predicted value of the transfer function using the estimated values of the parameters.

The observed values can be written as:

$$H(j\omega_i) = U_i + jV_i \quad (2)$$

and the predicted values can be written as:

$$\hat{H}(j\omega_i) = R_i(\theta) + jQ_i(\theta) \quad (3)$$

where θ represents the vector of parameters and the $R_i(\theta)$ and $Q_i(\theta)$ are real functions of these parameters and the frequency. These functions are given in Appendix A for the eight-parameter transfer function considered herein. Using equations 2 and 3, equation 1 can be written as:

$$\phi = \sum_{i=1}^{n} [U_i - R_i(\theta)]^2 + \sum_{i=1}^{n} [V_i - Q_i(\theta)]^2 \quad (4)$$

The main program requires that the sum of squares of residuals to be minimized be of the form

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1. Marquardt, D. W. An algorithm for least-squares estimation of nonlinear parameters. J Soc Indust Appl Math II (No. 2): 431-441 (1963).

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$$\Sigma\ Res^2 = \Sigma\ (\text{observed} - \text{function})^2 \ . \qquad (5)$$

In equation 4, the function is $R_i(\theta)$ for the real part and $Q_i(\theta)$ for the imaginary part. These two functions require different computations for the residual and different sets of partial derivatives to be evaluated. These functions and their partial derivatives with respect to the parameters are given in Appendix A for the eight-parameter transfer function.

Under the assumption that the real and imaginary parts of $H(j\omega_i)$ are independent for each ω_i and that the $H(j\omega_i)$ are independent for different ω, the problem of fitting a complex-valued function to n frequencies can be considered as a problem of fitting one of two real-valued functions to N = 2n independent data points. When only ensemble averaging is done to calculate the observed values of the transfer function, the approximate independence of the values at the Fourier frequencies is an immediate extension of the approximate independence for the periodogram. When tapering or smoothing is done, this will no longer be true, except for smoothed estimates at frequencies not using any common unsmoothed value. Therefore, ensemble averaging is the recommended method of obtaining the observed values. When only a single sample is available, the use of the original Bartlett window that involves dividing the sample into several subsamples of equal length and averaging the periodogram estimates from these subsamples is the recommended alternative.

The use of averaging still does not assure any reasonability of the assumption of independence of the real and imaginary parts at the same frequency. This appears to be analytically intractable to show, but preliminary results from some Monte Carlo simulation indicate that the assumption is probably not unreasonable.

Finally, the reasonableness of using equal weights at all frequencies should be considered. Assuming that the variances of the real and imaginary parts of all frequencies are equal, then equal weights should be used. Demonstrating equality of variances appears to be analytically intractable, although preliminary results from the simulation data suggest the assumption may be reasonably sound. Therefore, estimating the parameters of a transfer function by minimizing equation 4 and considering the 2n = N data values as independent with equal variances seems to be reasonable.

STRUCTURE OF THE SUBROUTINE

The required standard information available to the subroutine consists of the vector of parameter estimates from the previous iteration, the vector of N values of the dependent variable (Y), the matrix of N values of one or more independent variables (X), and the index of the

point whose residual and partial derivatives are currently being evaluated. The additional information needed for this estimation problem is whether the current value is a real part or imaginary part of an observed value. This is obtained by coding an extra independent variable, 1 if real and 2 if imaginary. Thus each of the N data vectors is made up of three quantities: the real or imaginary part of an observed value, the frequency in radians associated with the observed value, and an indicator of whether the data vector is for a real part or an imaginary part (coded 1 or 2).

Since the real and imaginary parts of the residuals and the partial derivatives are determined separately, the computations in the subroutine are done in two sections, one for the real part and the other for the imaginary part. Therefore, the subroutine is a two-function subroutine with an indicator to specify which function to use. An example of a subroutine which incorporates the ideas described above for the eight-parameter transfer function is shown in Appendix B.

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APPENDIX A

FUNCTIONS OF THE REAL AND IMAGINARY PARTS OF THE EIGHT-PARAMETER TRANSFER FUNCTION AND THEIR PARTIAL DERIVATIVES WITH RESPECT TO THE PARAMETERS

The transfer function can be written as:

$$\hat{H}(j\omega_i) = \frac{K[1+\gamma_1(j\omega_i) + \gamma_2\ (j\omega_i)^2 + \gamma_3\ (j\omega_i)^3]\ e^{-j\tau\omega_i}}{[1+\alpha_1(j\omega_i) + \alpha_2\ (j\omega_i)^2 + \alpha_3\ (j\omega_i)^3]}$$

Writing the exponential as:

$$e^{-j\tau\omega_i} = \cos \tau\omega_i - j \sin \tau\omega_i,$$

multiplying the numerator and denominator by the conjugate of the denominator, and collecting terms gives:

$$\hat{H}(j\omega_i) = R_i + jQ_i$$

where, dropping the i subscript,

$$R = K[(AB + CD) \cos \tau\omega + (AD-BC) \sin \tau\omega]/Z$$

$$Q = K[(AD - BC) \cos \tau\omega - (AB + CD) \sin \tau\omega]/Z$$

and

$$A = 1 - \alpha_2\omega^2$$

$$B = 1 - \gamma_2\omega^2$$

$$C = \omega(\alpha_1 - \alpha_3\omega^2)$$

$$D = \omega(\gamma_1 - \gamma_3\omega^2)$$

$$Z = A^2 + C^2$$

Denoting the partial derivatives of R and Q with respect to the parameter θ as $R|\theta$ and $Q|\theta$ and using the above defined terms, the partial derivatives are:

$R|K = R/K$

$R|\tau = K\omega[(AD - BC)\cos\tau\omega - (AB + CD)\sin\tau\omega]/Z$

$R|\gamma_1 = K\omega[C\cos\tau\omega + A\sin\tau\omega]/Z$

$R|\gamma_2 = K\omega^2[-A\cos\tau\omega + C\sin\tau\omega]/Z$

$R|\gamma_3 = K\omega^3[-C\cos\tau\omega - A\sin\tau\omega]/Z$

$R|\alpha_1 = \omega[K(D\cos\tau\omega - B\sin\tau\omega) - 2CR]/Z$

$R|\alpha_2 = \omega^2[K(-B\cos\tau\omega - D\sin\tau\omega) + 2AR]/Z$

$R|\alpha_3 = \omega^3[K(-D\cos\tau\omega + B\sin\tau\omega) + 2CR]/Z$

and

$Q|K = Q/K$

$Q|\tau = K\omega[-(AB + CD)\cos\tau\omega - (AD - BC)\sin\tau\omega]/Z$

$Q|\gamma_1 = K\omega[A\cos\tau\omega - C\sin\tau\omega]/Z$

$Q|\gamma_2 = K\omega^2[C\cos\tau\omega + A\sin\tau\omega]/Z$

$Q|\gamma_3 = K\omega^3[-A\cos\tau\omega + C\sin\tau\omega]/Z$

$Q|\alpha_1 = \omega[K(-B\cos\tau\omega - D\sin\tau\omega) - 2CQ]/Z$

$Q|\alpha_2 = \omega^2[K(-D\cos\tau\omega + B\sin\tau\omega) + 2AQ]/Z$

$Q|\alpha_3 = \omega^3[K(B\cos\tau\omega + D\sin\tau\omega) + 2CQ]/Z$

APPENDIX B

LISTING OF SUBROUTINE

The following subroutine is used in conjunction with our modified version of a program for least-squares estimation of nonlinear parameters. The section for the first key puts out the labeling for the full model form and sets up the test value for the indicator of real or imaginary part. The second key section estimates the function and the residual and the third key section estimates the partial derivatives.

```
      SUBROUTINE MODEL(KEY)
C  FITTING COMPLEX VALUED TRANSFER FUNCTION:  EQUAL WEIGHTS:
      IMPLICIT REAL*8(A-H,O-Z)
      COMMON X(300,10),Y(300),B(30),P(30),PRNT(5),HDR2(18),F,RES,NI(40),
     1 I,N,K,IP,NPRNT
      DIMENSION XHDR(18)
      DATA XHDR/144HMODEL FOR FITTING IN THE FREQUENCY DOMAIN;S=J OMEGA
     1                   H(S)=K(1+G(1)S+...+G(3)S**3)EXP(-TS) / (1+A(1)
     2 S+...+A(3)S**3)              /
      GO TO (10,20,30), KEY
   10 DO 5 I=1,18
    5 HDR2(I)=XHDR(I)
      REAL=1.DO
      RETURN
C  B(1)=K
C  B(2)=T
C  B(3)=G(1)
C  B(4)=G(2)
```

```
C  B(5)=G(3)
C  B(6)=A(1)
C  B(7)=A(2)
C  B(8)=A(3)
   20 W2=X(I,1)**2
      TW=B(2)*X(I,1)
      A=1.DO-B(7)*W2
      E=1.DO-B(4)*W2
      C=X(I,1)*(B(6)-B(8)*W2)
      D=X(I,1)*(B(3)-B(5)*W2)
      Z=A**2+C**2
      CS=DCOS(TW)
      SN=DSIN(TW)
      ABCD=A*E+C*D
      ADBC=A*D-E*C
      IF(X(I,2).GT.REAL) GO TO 25
      F=B(1)*(ABCD*CS+ADBC*SN)/Z
      RES=(Y(I)-F)
      RETURN
   25 F=B(1)*(ADBC*CS-ABCD*SN)/Z
      RES=(Y(I)-F)
      RETURN
   30 W=X(I,1)
      W3=W*W2
     PK=B(1)
```

```
      IF(X(I,2).GT.REAL) GO TO 35
      P(1)=F/PK
      P(2)=PK*W*(ADBC*CS-ABCD*SN)/Z
      P(3)=PK*W*(C*CS+A*SN)/Z
      P(4)=PK*W2*(C*SN-A*CS)/Z
      P(5)=PK*W3*(-C*CS-A*SN)/Z
      P(6)=W*(PK*(D*CS-E*SN)-2.DO*C*F)/Z
      P(7)=W2*(PK*(-E*CS-D*SN)+2.DO*A*F)/Z
      P(8)=W3*(PK*(-D*CS+E*SN)+2.DO*C*F)/Z
      RETURN
   35 P(1)=F/PK
      P(2)=PK*W*(-ADBC*SN-ABCD*CS)/Z
      P(3)=PK*W*(A*CS-C*SN)/Z
      P(4)=PK*W2*(C*CS+A*SN)/Z
      P(5)=PK*W3*(-A*CS+C*SN)/Z
      P(6)=W*(PK*(-E*CS-D*SN)-2.DO*C*F)/Z
      P(7)=W2*(PK*(-D*CS+E*SN)+2.DO*A*F)/Z
      P(8)=W3*(PK*(E*CS D*SN)+2.DO*C*F)/Z
      RETURN
      END
```